# The University of Alabama in Huntsville Final Report

EXAMINATION OF VARIOUS TURBULENCE MODELS FOR APPLICATION IN LIQUID ROCKET THRUST CHAMBERS

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NASA Contract Number: NAS8-36955

/Delivery Order Number 38

April 30, 1991

ASA-CR-184406) EXAMINATION OF RIGUS TURBULENCE MODELS FOR

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#### Abstract

There is a large variety of turbulence models available. models include direct numerical simulation, large eddy simulation, Reynolds stress/flux model, zero equation model, one equation model, two equation  $\tilde{k}-\tilde{\epsilon}$  model, multiple-scale model, etc. Each turbulence model contains different physical assumptions and requirements. natures of turbulence are randomness, irregularity, diffusivity and dissipation. In this study, the capabilities of the turbulence models, including physical strength, weakness, limitations, as well as numerical and computational considerations, have been reviewed. Recommendations are made for the potential application of a turbulence model in thrust chamber and performance prediction programs. In this study, the full Reynolds stress model is In a workshop, specifically called for the assessment recommended. of turbulence models for application in liquid rocket thrust chambers, most of the experts present were also in favor of the recommendation of the Reynolds stress model.

#### I. Introduction

Turbulence consists of random velocity fluctuations, so in principle, it must be treated with statistical methods. Turbulent momentum fluxes and turbulent diffusion fluxes are usually much greater than the mean molecular length scale in the turbulent regime. However, the turbulent length scale of the excited modes still remains within the band of computationally resolved grids (either in the physical or spectral domain). This restriction imposes a severe limitation on the development of the direct numerical simulation method representing turbulent flows even with the advancement of in addition to present day supercomputer technology, consideration of the mathematical description of reactive flow transport due to the randomness in the fields of velocity and thermochemical fluctuations (Givi, 1989; 1990). In other words, assuming that the direct computation of the usual thermochemical balance equations can be carried out with the help of much better supercomputers, it is still impossible in practice to accomplish the computation of every realization of this ensemble of flow fields, even if we are satisfied simply with a brute numerical method (Borghi, 1988).

The nature of turbulence covers a wide spectrum of turbulent energy transports in which turbulent energy production is associated with smaller wave numbers; while turbulent energy dissipation is attached to larger wave numbers. In other words, turbulence consists of fluctuations of motions varying continuously with a spectrum of

length and time scales. It is obvious that any turbulence closure model with a single length scale can not properly cover the transition of turbulent energy from the production end to the dissipation end.

Thermochemical and dynamical flow fields of liquid rocket thrust chambers are highly irregular and random in nature. Proper selection of the best turbulence model is the key to understanding the characterisitics of reacting flow fields.

Turbulence models available include model-free simulations (including large eddy simulation), which is a direct numerical simulation of thermochemical flow fields, and turbulence closure models which apply Favre and Reynolds averages on flow fields with random fluctuations. Turbulence closure models can be further divided into the models which do and do not adopt the concept of Boussinesq's expression. By adopting the concept of Boussinesg's expression, Reynold stress and diffusion fluxes become eddy viscosity and eddy diffusion fluxes repectively, which assume that the flow fields are in the form of isotropic turbulence. This approach has produced formulations which are known as: zero equation, one equation, two equation (including  $\tilde{k}-\tilde{\epsilon}$  model), and multi-scale turbulence models. Reynolds stress/flux models were developed by the direct derivation of Reynolds stress/diffusion fluxes from the mean value balance equations of continuity, momentum, energy and species concentration, instead of using eddy viscosity/eddy diffusion flux concepts from Boussinesq's expression. Reynolds stress/flux models also include algebraic stress/flux and multiscale turbulence.

With this large variety of turbulence models available, the present report discusses the advantages and disadvantages of applying these models in the reacting flow calculation, in particular the suitability for random flow field computations within a liquid rocket thrust chamber.

Please note that some text in this report is repetitive for the sole purpose of convenience to the reader and to emphasize the importance of the topic in question.

# II. Formulations of Turbulent Flows in Reacting Fluids

It is now common to consider a turbulent flow as an ensemble of random flow fields. This includes the following considerations:

(1) each of these fields does satisfy the classical thermodynamical balance equations with a particular set of initial and boundary conditions; (2) each field is different due to the differences in initial and boundary conditions; and (3) each flow can be very different because the sensitivity to boundary conditions is quite large. This <u>Turbulent Regime</u> occurs very often when a characteristic Reynolds number (a ratio of convective force to viscous force) is large enough. Other types of instabilities leading to <u>Turbulence</u> which are characterized by other numbers could occur, especially for reacting flows where highly non-linear terms appear in the equations.

Assuming that the thermochemical balance equations are valid, it is still impossible to compute these flow fields even if we settle for a brute numerical method (Borghi, 1988). The time scales and length scales, that we know to exist within the turbulent regime of reacting flows, are so small with respect to the time or length scales of interest that we would need an incredibly large computer memory capacity and an enormous amount of computer time. In addition the computation of just one or two realizations would be of no interest, and we would not be able to perform computer experiments with the same initial and boundary conditions. Indeed, only statistical quantities are of practical meaning in order to describe the randomness within the flow. In other words, we first need mean

values, then variance and correlations, and also probability density functions.

The method of approach due to Reynolds just described, has been applied for cases of non-reacting turbulent flows as early as 1890. Mean values for the components of the fluid velocity, the pressure or the concentration of diffusing species, and also the variance and correlations of the velocity fluctuations and other flow parameters have been defined mathematically as well as experimentally (Tennekes and Lumley, 1972).

Due to the variations and fluctuations of the fluid density which are more likely to occur in reacting flows with large temperature gradients, it is now common in turbulent combustion studies to change the classical definition a little. It appears that the use of mean values, weighted by the density  $\rho$ , is more appropriate to handle fluid flows with a nature of randomness, irregularity, diffusivity and dissipation.

Let us consider a reacting flow with a velocity component in  $\alpha$  direction,  $u_{\alpha}$ ; density,  $\rho$ ; pressure, P; temperature, T; enthalpy, h; viscous stress tensor along  $\alpha$  and  $\beta$  directions,  $\tau_{\alpha\beta}$ ; external force, such as gravitational acceleration in  $\alpha$  direction,  $g_{\alpha}$ ; heat flux in  $\alpha$  direction,  $g_{\alpha}$ ; and mass fraction of species s,  $Y_{s}$ . The four governing equations of continuity, momentum, energy, and species can be expressed as follows:

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_{\alpha}} (\rho u_{\alpha}) = 0 \qquad \alpha = 1, 2, 3 \qquad (2-1)$$

Momentum Equation:

$$\frac{\partial}{\partial t} (\rho u_{\alpha}) + \frac{\partial}{\partial x_{\beta}} (\rho u_{\alpha} u_{\beta}) = \rho g_{\alpha} - \frac{\partial P}{\partial x_{\alpha}} + \frac{\partial \tau_{\alpha\beta}}{\partial x_{\beta}}$$
 (2-2)

Energy Equation:

$$\frac{\partial}{\partial t} \left[ \rho \left( h - \frac{P}{\rho} + \frac{1}{2} u_{\beta} u_{\beta} \right) \right] + \frac{\partial}{\partial x_{\beta}} \left[ \rho u_{\beta} \left( h - \frac{P}{\rho} + \frac{1}{2} u_{\beta} u_{\beta} \right) \right] + \frac{\partial}{\partial x_{\beta}} \left( \pi_{\alpha \beta} u_{\alpha} \right) - \frac{\partial q_{\beta}}{\partial x_{\beta}}$$

$$+ \frac{1}{2} u_{\beta} u_{\beta} \right] = \rho u_{\beta} q_{\beta} - \frac{\partial}{\partial x_{\beta}} (\pi_{\alpha \beta} u_{\alpha}) - \frac{\partial q_{\beta}}{\partial x_{\beta}}$$
(2-3)

Species Equation:

$$\frac{\partial}{\partial t} (\rho Y_s) + \frac{\partial}{\partial x_{\beta}} (\rho Y_s u_{\beta}) = -\frac{\partial}{\partial x_{\beta}} (\rho Y_s u_{s\beta}) + W_s \qquad (2-4)$$

where  $\mathbf{u}_{s\beta}$  is the diffusion velocity of species s in  $\beta$  direction.

In these expressions, viscous stress tensor,  $\tau_{\alpha\beta}$ ; stress tensor,  $\pi_{\alpha\beta}$ ; and heat flux,  $q_{\alpha}$ , can be shown in the following forms:

$$\tau_{\alpha\beta} = \left(\frac{\partial u_{\alpha}}{\partial x_{\beta}} + \frac{\partial u_{\beta}}{\partial x_{\alpha}}\right) - \frac{2}{3} \mu \left(\frac{\partial u_{k}}{\partial x_{k}}\right) \delta_{\alpha\beta}$$
 (2-5)

$$\pi_{\alpha\beta} = P \delta_{\alpha\beta} - \tau_{\alpha\beta} \tag{2-6}$$

$$q_{\alpha} = -k_{th} \frac{\partial T}{\partial x_{\alpha}} + \rho \sum_{s} (Y_{s}h_{s}u_{s\alpha}) + q_{\alpha}^{D}$$
 (2-7)

where  $q_{\alpha}^D$  represents the sum of the Dufour heat flux and radiative heat flux;  $k_{t\,h}$ , the thermal conductivity; and  $W_s$ , the chemical reaction rate of species s.

To obtain mean values of the thermochemical balance equation, density weighted values (or Favre mean values) are used for velocity components  $(u_{\alpha})$ , temperature (T), mass fraction  $(Y_{\epsilon})$ , and enthalpy (h), while the conventional mean values (or Reynolds mean values) are kept for pressure (P) and density  $(\rho)$ .

The conventional mean values are defined as

$$A = \overline{A} + A' \tag{2-8}$$

where () is the conventional mean value; and ()', the corresponding value for fluctuation. The density weighted mean values are defined as

$$\mathbf{A} = \tilde{\mathbf{A}} + \mathbf{A''} \tag{2-8}$$

where () is the density weighted mean value; and ()", the corresponding value of fluctuation. Detailed mathematical expressions for both conventional and density weight mean values are discussed in Appendix A.

The mean value balance equations for continuity, momentum, energy, and species concentration can be shown as follows:

Continuity Equation:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_{\alpha}} \left( \overline{\rho u_{\alpha}} \right) = 0 \tag{2-9}$$

Momentum Equation:

$$\frac{\partial}{\partial t} \left( \stackrel{\sim}{\rho u_{\alpha}} \right) + \frac{\partial}{\partial x_{\beta}} \left( \stackrel{\sim}{\rho u_{\alpha}} \stackrel{\sim}{u_{\beta}} \right) = \stackrel{\sim}{\rho} g_{\alpha} - \frac{\partial \overline{P}}{\partial x_{\alpha}} + \frac{\partial}{\partial x_{\beta}} \left( \stackrel{\sim}{\tau_{\alpha\beta}} \right)$$

$$- \stackrel{\sim}{\rho u_{\alpha}} \stackrel{\parallel}{u_{\beta}}$$
(2-10)

Energy Equation:

$$\frac{\partial}{\partial t} \left[ -\frac{1}{\rho} \left( \widetilde{h} + \frac{1}{2} \widetilde{u}_{\alpha} \widetilde{u}_{\alpha} + \frac{1}{2} \widetilde{u}_{\alpha} \widetilde{u}_{\alpha}^{"} \right) \right] + \frac{\partial}{\partial x_{\alpha}} \left[ -\widetilde{\rho} \widetilde{u}_{\alpha} \left( \widetilde{h} + \frac{1}{2} \widetilde{u}_{\alpha} \widetilde{u}_{\alpha}^{"} + \frac{1}{2} \widetilde{u}_{\alpha}^{"} \widetilde{u}_{\alpha}^{"} \right) \right] + \frac{\partial}{\partial x_{\alpha}} \left[ -\widetilde{\rho} \widetilde{u}_{\alpha} \left( \widetilde{h} + \frac{1}{2} \widetilde{u}_{\alpha} \widetilde{u}_{\alpha}^{"} \right) \right] + \frac{\partial}{\partial u_{\alpha}} \widetilde{u}_{\alpha}^{"} + \frac{\partial}{\partial u_{\alpha}} \widetilde{u}_{\alpha}^{"} \widetilde{u}_{\alpha}^{"} \widetilde{u}_{\alpha}^{"} \right] + \frac{\partial}{\partial u_{\alpha}} \left[ -\widetilde{\rho} \widetilde{u}_{\alpha} \widetilde{u}_{\alpha}^{"} \widetilde{u}_{\alpha}^{"} \right] + \frac{\partial}{\partial u_{\alpha}} \widetilde{u}_{\alpha}^{"} + \frac{\partial}{\partial u_{\alpha}} \left( -\widetilde{\tau}_{\alpha} \widetilde{u}_{\alpha} \widetilde{u}_{\alpha}^{"} \right) + \frac{\partial}{\partial u_{\alpha}} \widetilde{u}_{\alpha}^{"} \right] + \frac{\partial}{\partial u_{\alpha}} \widetilde{u}_{\alpha}^{"} + \frac{\partial}{$$

Species Equation:

$$\frac{\partial}{\partial t} \left( \stackrel{\sim}{\rho Y_s} \right) + \frac{\partial}{\partial x_{\alpha}} \left( \stackrel{\sim}{\rho Y_s} \stackrel{\sim}{u_{\alpha}} + \stackrel{\sim}{\rho Y_s} \stackrel{"}{u_{\alpha}} \right) \\
= - \frac{\partial}{\partial x_{\alpha}} \left( \stackrel{\sim}{\rho Y_s} \stackrel{\sim}{u_{s\alpha}} + \stackrel{\sim}{\rho Y_s} \stackrel{"}{u_{s\alpha}} \right) + \stackrel{\sim}{W_s}$$
(2-12)

where  $u_{s\alpha}$  is the diffusion velocity of species s in  $\alpha$  direction. In these manipulations, the following relations have been used:

$$\tau_{\alpha\beta} = \overline{\tau}_{\alpha\beta} + \tau_{\alpha\beta}' \tag{2-13}$$

$$q_{\alpha} = \overline{q}_{\alpha} + q_{\alpha}' \tag{2-14}$$

$$\overline{\tau}_{\alpha\beta} = \overline{\mu} \left( \frac{\partial \widetilde{u}_{\alpha}}{\partial x_{\beta}} + \frac{\partial \widetilde{u}_{\beta}}{\partial x_{\alpha}} \right) + \overline{\mu} \left( \frac{\partial \overline{u}_{\alpha}^{\mu}}{\partial x_{\beta}} + \frac{\partial \overline{u}_{\beta}^{\mu}}{\partial x_{\alpha}} \right)$$

$$+ \mu' \left( \frac{\partial u''_{\alpha}}{\partial x_{\beta}} + \frac{\partial u''_{\beta}}{\partial x_{\alpha}} \right) - \frac{2}{3} \left( \overline{u} \frac{\partial \overline{u}_{k}}{\partial x_{k}} + \overline{u} \frac{\partial \overline{u}''_{k}}{\partial x_{k}} \right)$$

$$+ \mu' \frac{\partial u_k''}{\partial x_k} \right) \delta_{\alpha\beta}$$
 (2-15)

$$\mu = \overline{\mu} + \mu' \tag{2-16}$$

$$\tau_{\alpha\beta} = \mu' \left( \frac{\partial \widetilde{u}_{\alpha}}{\partial x_{\beta}} + \frac{\partial \widetilde{u}_{\beta}}{\partial x_{\alpha}} \right) - \frac{2}{3} \mu' \left( \frac{\partial \widetilde{u}_{k}}{\partial x_{k}} \right) \delta_{\alpha\beta}$$
 (2-17)

$$\overline{q}_{\alpha} = -\left(\overline{k}_{th} \frac{\partial \widetilde{T}}{\partial x_{\alpha}} + \overline{k}_{th} \frac{\partial \widetilde{T''}}{\partial x_{\alpha}} + k_{th} \frac{\partial \widetilde{T''}}{\partial x_{\alpha}} + k_{th} \frac{\partial \widetilde{T''}}{\partial x_{\alpha}}\right) + - \sum_{s} \widetilde{Y}_{s} \widetilde{h}_{s} \widetilde{u}_{s\alpha}$$
(2-18)

$$+ \widetilde{Y_{s}h_{s}''u_{s\alpha}''} + \widetilde{Y_{s}'h_{s}''u_{s\alpha}} + \widetilde{u_{s\alpha}''Y_{s}''h_{s}} + \widetilde{Y_{s}''h_{s}''u_{s\alpha}''} + \widetilde{q_{k}'}$$
 (2-19)

$$q_{\alpha}' = -k_{th} \frac{\partial T}{\partial x_{\alpha}} + \rho_{s}^{\Sigma} (h_{s}Y_{s}u_{s\alpha} + Y_{s}h_{s}u_{s\alpha} + u_{s\alpha}Y_{s}h_{s})$$

$$+ q_{\alpha}^{\mathfrak{D}'}$$
 (2-20)

For the purpose of numerically solving turbulent reacting flows, one has to solve the mean value balance equations of continuity, momentum, energy, and species concentration, shown in Equations (2-9) to (2-12), in conjunction with the mean value equation of state  $\overline{P} = - \overbrace{\rho RT}$  (2-21)

Careful examination of Equations (2-9) to (2-12) indicate that turbulent diffusion fluxes contain  $u_{\alpha}^{il}$   $u_{\beta}^{il}$ ,  $u_{\alpha}^{il}$   $Y_{s}^{il}$ , and  $u_{\alpha}^{il}$   $h^{il}$  terms which are usually much larger than the mean molecular length and time scale in the turbulent regime, and also involve correlations between fluctuations, and certainly not the mean values only (see Appendix for description). Unless turbulent diffusion fluxes are well defined, it is very difficult to obtain a closed form solution numerically. In other words, the study of turbulence becomes a closure problem in which the modeling of turbulent diffusion fluxes must be predetermined before one can solve the turbulent reacting flow problem

numerically.

# III. Time Scale and Length Scale of Turbulence

The mean balance equations of continuity, momentum, energy and species, shown in Equations (2-9), (2-10), (2-11) and (2-12), respectively, can not be used directly for solving turbulent reacting flow problems. These equations involve new quantities of the turbulent Reynolds stress/diffusion fluxes, such as  $u_{\alpha}^{\prime\prime}u_{\beta}^{\prime\prime}$ ,  $u_{\alpha}^{\prime\prime}Y_{s}^{\prime\prime}$  and  $u_{\alpha}^{\prime\prime}h_{s}^{\prime\prime}$ , which are usually much greater than the mean molecular scale in the turbulent regime, and also correlations between fluctuations which are not mean values only.

The modeling of the turbulent diffusion fluxes generally follow Boussinesq's expression resulting in the following closure assumption:

$$-\frac{\widetilde{u_{\alpha}u_{\beta}}}{\widetilde{u_{\alpha}u_{\beta}}} = \mu_{t} \left( \frac{\widetilde{\partial u_{\alpha}}}{\partial x_{\beta}} + \frac{\widetilde{\partial u_{\beta}}}{\partial x_{\alpha}} \right) - \frac{2}{3} \delta_{\alpha\beta} \left( \frac{-\widetilde{k}}{\rho \widetilde{k}} + \mu_{t} \frac{\widetilde{\partial u_{k}}}{\partial x_{k}} \right)$$
(3-1)

$$-\frac{1}{\rho} \underbrace{\mathbf{u}_{\alpha}^{"} \mathbf{Y}_{s}^{"}}_{\mathbf{S} \mathbf{c}_{t}} = \frac{\mathbf{u}_{t}}{\mathbf{S} \mathbf{c}_{t}} \underbrace{\frac{\partial \widehat{\mathbf{Y}_{s}}}{\partial \mathbf{x}_{\alpha}}}_{\mathbf{S} \mathbf{c}_{t}}$$
(3-2)

$$-\frac{1}{\rho} \underbrace{\mathbf{u}_{\alpha}^{\mu} \mathbf{h}^{\mu}}_{\mathbf{pr}_{+}} = \frac{\mathbf{u}_{t}}{\mathbf{pr}_{+}} \underbrace{\frac{\partial \widetilde{\mathbf{h}}}{\partial \mathbf{x}_{\alpha}}}_{\mathbf{q}_{\alpha}}$$
(3-3)

where  $\tilde{k} = 1/2$   $u_{\alpha}^{\mu}u_{\alpha}^{\mu}$  is the turbulent kinetic energy;  $\mu_t$ , the eddy viscosity;  $Sc_t$ , the turbulent Schmidt number; and  $Pr_t$ , the turbulent Prandtl number. It is noted that  $\mu_t$  is <u>not</u> a property of the fluid. In fact, experiments show in particular that  $Sc_t$  and  $Pr_t$  are independent of the nature of the species, and therefore  $\mu_t$  has to be a property of the turbulent flow. In other words,  $\mu_t$  does depend on a length scale and a time scale of the turbulence. This can be shown as

follows with modification from Equation (3-1):

$$\frac{\underline{u}_{t}}{\rho} = \frac{-(\underline{u}_{\alpha}^{"}\underline{u}_{\beta}^{"})_{m}}{\left(\frac{\partial \widetilde{u}_{\alpha}}{\partial x_{\beta}} + \frac{\partial \widetilde{u}_{\beta}}{\partial x_{\alpha}}\right)_{m}} = \frac{-(\underline{u}_{\alpha}^{"}\underline{u}_{\beta}^{"})^{1/2}}{\left(\frac{\partial \widetilde{u}_{\alpha}}{\partial x_{\beta}} + \frac{\partial \widetilde{u}_{\beta}}{\partial x_{\alpha}}\right)_{m}} \quad (\underline{u}_{\alpha}^{"}\underline{u}_{\beta}^{"})^{1/2} \tag{3-4}$$

(Length Scale) (Velocity Scale)

subscript m denotes that the quantity is evaluated where  $u_{\alpha}^{"}u_{\beta}^{"}$  is a maximum value.

Kolmogoroff suggests that at sufficiently high Reynolds numbers there is a range of high wave numbers where the turbulence is statistically in equilibrium and uniquely determined by the parameters of viscous dissipation of turbulent motions,  $\epsilon$ , and kinematic viscosity,  $\nu (= \mu/\rho)$  (Hinze, 1975). This state of equilibrium is <u>universal</u>. This equilibrium range is termed "universal" because the turbulence in this range is independent of external conditions, and any change in the effective length scale and time scale of this turbulence can only be a result of the effect of the parameters  $\epsilon$  and  $\nu$ . The Kolmogoroff length scale,  $\eta_k$ , time scale,  $\tau_k$ , and velocity scale,  $\nu_k$ , are represented by:

$$\eta_k = \left(\frac{\gamma^3}{\epsilon}\right)^{1/4} \tag{3-5}$$

$$\tau_k = \left(\frac{\nu}{\epsilon}\right)^{1/2} \tag{3-6}$$

$$\mathbf{v}_{k} = (\gamma \, \epsilon)^{1/4} \tag{3-7}$$

The eddy wave number,  $k_d$ , where the viscous effects become very strong will be of the same order as  $1/\eta_k$ .  $k_d$  is defined as:

$$k_d = \frac{1}{\eta_k} = \left(\frac{\epsilon}{v^3}\right)^{1/4} \tag{3-8}$$

In other words, the viscous effect becomes much stronger than the turbulent dissipation when the eddy wave number is much greater than k<sub>d</sub>.

Viscous dissipation of turbulent motion is expressed as:

$$\tilde{\epsilon} = v \frac{\partial u_{\alpha}^{\mu}}{\partial x_{\beta}} \left( \frac{\partial u_{\alpha}^{\mu}}{\partial x_{\beta}} + \frac{\partial u_{\beta}^{\mu}}{\partial x_{\alpha}} \right)$$
 (3-9)

For the case of homogeneous turbulence in which all spatial derivatives of mean turbulent quantities become zero, the viscous dissipation of turbulent motion becomes:

$$\tilde{\epsilon} = \gamma \left( \frac{\partial u_{\alpha}^{"}}{\partial x_{\beta}} \right)^{2} \tag{3-10}$$

Definitions for the turbulent velocity scale  $V_t$ , integral length scale  $\lambda_i$ , and Taylor micro-length scale  $\lambda_t$  applied to subsequent terms yield:

$$\widetilde{\mathbf{u}_{\alpha}^{\mu}\mathbf{u}_{\beta}^{\mu}} \sim \mathbf{V}, \tag{3-11}$$

$$\widetilde{\mathbf{u}_{\alpha}^{\mu}\mathbf{u}_{\beta}^{\mu}} \left( \frac{\partial \widetilde{\mathbf{u}_{\alpha}}}{\partial \mathbf{x}_{\alpha}} + \frac{\partial \widetilde{\mathbf{u}_{\beta}}}{\partial \mathbf{x}_{\beta}} \right) \sim \frac{\mathbf{v_{t}}^{3}}{\lambda_{t}}$$
(3-12)

$$\frac{\widetilde{u_{\alpha}^{\mu}u_{\beta}^{\mu}}\left(\frac{\partial \widetilde{u_{\alpha}}}{\partial x_{\alpha}} + \frac{\partial \widetilde{u_{\beta}}}{\partial x_{\beta}}\right) \sim \frac{V_{t}^{3}}{\lambda_{t}}}{\frac{\partial u_{\alpha}^{\mu}}{\partial x_{\beta}}\left(\frac{\partial u_{\alpha}^{\mu}}{\partial x_{\alpha}} + \frac{\partial u_{\beta}^{\mu}}{\partial x_{\beta}}\right) \sim \frac{V_{t}^{2}}{\lambda_{t}^{2}}}$$
(3-12)

$$\frac{\partial}{\partial x_{\beta}} \underbrace{(u_{\alpha}''u_{\beta}'')}_{\lambda_{i}} \sim \frac{V_{t}^{3}}{\lambda_{i}}$$
(3-14)

where Equation (3-11) shows density-weighted Reynolds stress; Equation (3-12), turbulence production by density-weighted Reynolds stress; Equation (3-13), viscous dissipation of turbulent energy by Comparison of length scales indicates:

 $\lambda_i \gg \lambda_T \gg \eta_k$  viscous dissipation (3-15) where  $\lambda_i$ ,  $\lambda_T$ , and  $\eta_k$  denote integral length, Taylor micro-length, and Kolmogoroff length scales, respectively. Equation (3-15) shows a cascade transport of turbulent energy in which large inhomogeneous eddies transport energy to small homogeneous eddies, which finally disappear through viscous dissipation.

## IV. Examination of Various Turbulence Models

In the previous section, we have indicated that the diffusion fluxes,  $\overrightarrow{u'_{\alpha}u'_{\beta}}$ ,  $\overrightarrow{u'_{\alpha}y''_{\beta}}$  and  $\overrightarrow{u'_{\alpha}h''}$  obtained from density-weighted mean values of the balance equations, require a specification for the closure problem. By using Boussinesq's eddy viscosity model, it is evident that eddy viscosity  $v_t$  is not a property of the fluid, but is simply a function of a length scale and a time scale of the turbulence. It also has been shown in the previous section that there are various length scales of turbulence, which come from the inhomogenous large eddy integral length scale, Taylor microscale and a homogenous small eddy Kolmogoroff length scale, before viscous dissipation becomes effective in energy dissipation.

There are several ways to model the eddy viscosity  $\nu_{\rm t}$  before one can solve the turbulent reacting flow by means of satisfying the closure problem.

#### (A) Zero Equation Models

Zero equation models are mostly based on the eddy viscosity concept. This concept uses the mathematical convenience of retaining the same form of differential equations for laminar and turbulent flows and allowing the use of the same solution procedure.

The first turbulence model proposed, Prandtl's mixing length hypothesis, is still widely used. It employs the eddy viscosity concept which relates the turbulent transport terms to the local gradient of mean flow quantities, namely:

$$\widetilde{\mathbf{u}_{\alpha}^{"}\mathbf{u}_{\beta}^{"}} = -\mathbf{v}_{t} \left( \frac{\partial \widetilde{\mathbf{u}_{\alpha}}}{\partial \mathbf{x}_{\beta}} + \frac{\partial \widetilde{\mathbf{u}_{\beta}}}{\partial \mathbf{x}_{\alpha}} \right)$$
(4-1)

where v<sub>t</sub> is the eddy viscosity.

The Prandtl mixing length hypothesis calculates the distribution of eddy viscosity by relating it to the mean velocity gradient

$$v_{t} = C_{\mu}L_{m}^{2} \left[ \left( \frac{\partial \widetilde{u}_{\alpha}}{\partial x_{\beta}} + \frac{\partial \widetilde{u}_{\beta}}{\partial x_{\alpha}} \right) \right]$$
 (4-2)

This relation involves a single unknown parameter, the mixing length  $L_m$  whose distribution over the flow field has to be prescribed with an empirical information.  $C_\mu$  is a constant . The mixing length model has been used for thin shear layers and wall boundary layers (Spalding, 1982). The main drawback with this model is the evaluation of  $L_m$  for different types of turbulent flows. The evaluation of  $L_m$  becomes difficult for recirculating flows, three dimensional flows, reacting flows, etc. In the already empirical specification of the mixing length , it is difficult to incorporate in any useful manner, the effects of curvature, buoyancy, rotation, etc. The transport and memory effects of turbulence are not accounted for in the mixing length model because transport equations for turbulent quantities are not involved in this model.

#### (B) One Equation Models

One of the simplest ways to characterize the turbulence is to consider the eddy viscosity in terms of two quantities,  $\lambda_i$  its integral length scale and  $\tilde{k}$  its kinetic energy (the time scale is nothing but  $\lambda_i/k^{1/2}$ ). Eddy viscosity by dimensional analysis

becomes:

$$v_{t} = C_{\mu} \lambda_{i} k^{1/2} \tag{4-3}$$

The integral length scale is specified algebraically and hence is turbulent flow dependent. The turbulent kinetic energy is derived from the Navier-Stokes equations in the one equation model by solving its transport properties (Launder and Spalding, 1972). This approach performs only marginally better than the zero equation model in terms of the modeling of recirculating flows, three dimensional flows, reacting flows, etc.

### (C) Two Equation Models

In attempts to eliminate the need for specifying the turbulent length scale as a function of position throughout the flow, the eddy viscosity, shown in Equations (4-2) and (4-3), can be replaced by the following equation:

$$v_{t} = C_{\mu} \frac{\tilde{k}^{2}}{\tilde{\epsilon}} \tag{4-4}$$

In this expression,  $C_{\mu}$  is a scalar constant for isotropic turbulence and becomes a vector quantity (no longer a constant value) for the marginal extension to cover the cases of anisotropic turbulence, such as three-dimensional rotation flows. The eddy viscosity can be determined if one can solve two differential equations, one for the density weighted mean values of turbulent kinetic energy  $\tilde{k}$  and the other one for the density weighted mean value of turbulent dissipation  $\tilde{\ell}$ .

The modeled equations for  $\tilde{k}$  and  $\tilde{\epsilon}$  are given below: Kinetic Energy  $(\tilde{k})$  Equation:

$$\frac{\partial}{\partial t} \left( \overline{\rho} \ \widetilde{k} \right) + \frac{\partial}{\partial x_{\alpha}} \left( \overline{\rho} \ \widetilde{u}_{\alpha} \ \widetilde{k} \right) = \widetilde{P}_{k} + \frac{\partial}{\partial x_{\alpha}} \left[ \frac{u_{t}}{Pr_{t}} \frac{\partial \widetilde{k}}{\partial x_{\alpha}} \right] + \frac{u_{t}}{\overline{\rho}^{2} Pr_{t}} \frac{\partial \overline{\rho}}{\partial x_{\alpha}} \frac{\partial \overline{P}}{\partial x_{\alpha}} - \overline{\rho} \ \widetilde{\epsilon}$$

$$(4-5)$$

Kinetic Energy Dissipation  $(\epsilon)$  Equation:

$$\frac{\partial}{\partial t} \left( \frac{\partial}{\rho \epsilon} \right) + \frac{\partial}{\partial x_{\alpha}} \left[ \frac{\partial}{\rho} \widetilde{u}_{\alpha} \widetilde{\epsilon} \right] = C \epsilon_{1} \frac{\widetilde{\epsilon}}{\widetilde{k}} \widetilde{P}_{k} - C_{\epsilon_{1}} \frac{\widetilde{\epsilon}}{\widetilde{k}} \frac{\mu_{t}}{\overline{\rho}^{2} \operatorname{Pr}_{t}} \frac{\partial \overline{\rho}}{\partial x_{\alpha}} \frac{\partial \overline{P}}{\partial x_{\alpha}} + \frac{\partial}{\partial x_{\alpha}} \left[ \frac{\mu_{t}}{\sigma_{\epsilon}} \frac{\partial \widetilde{\epsilon}}{\partial x_{\alpha}} \right] - C_{\epsilon_{2}} \frac{\overline{\epsilon}^{2}}{\widetilde{k}}$$

$$(4-6)$$

where

$$\tilde{\mathbf{k}} = \frac{1}{2} \underbrace{\mathbf{u}_{\alpha}^{\prime\prime} \mathbf{u}_{\alpha}^{\prime\prime}}_{\mathbf{a}} \tag{4-7}$$

$$\tilde{\epsilon} = y \left(\frac{\partial \tilde{u}_{\alpha}^{ii}}{\partial x_{\alpha}}\right)^{2} \tag{4-8}$$

$$\tilde{P}_{k} = -\frac{1}{\rho} \underbrace{\tilde{u}_{\alpha}^{"} \tilde{u}_{\beta}^{"}}_{\partial x_{\beta}} \frac{\partial \tilde{u}_{\alpha}}{\partial x_{\beta}}$$
(4-9)

The coefficients, such as  $C_{\epsilon 1}$ ,  $C_{\epsilon 2}$ ,  $\sigma_{\epsilon}$ , are constants in the sense that they are not changed in the modeling calculation. However, these constants need to be changed in order to accommodate the effects such as curvature, low Reynolds number, near wall effects, etc.  $Pr_t$  is the turbulent Prandtl number which is not species dependent, and is also considered a constant in the modeling calculation.

Libby (1976), Bilger (1976), and Jones (1980), and Bray et al., (1981)

have devoted particular attention to this problem. The modified balance equations for turbulent kinetic energy and dissipation rate of turbulence can be shown as follows:

Modified Turbulent Kinetic Energy Equation:

$$\frac{\partial}{\partial t} = \frac{\partial}{\rho \hat{k}} + \frac{\partial}{\partial x_{\alpha}} = \frac{\partial}{\partial x_{\alpha}} \left( -\frac{\rho}{2} u_{\alpha}^{"} u_{\beta}^{"} u_{\beta}^{"} + p' u_{\alpha}^{"} \right)$$

$$-\frac{\partial}{\rho} u_{\alpha}^{"} u_{\beta}^{"} \frac{\partial u_{\beta}^{"}}{\partial x_{\alpha}} - u_{\beta}^{"} \frac{\partial \overline{P}}{\partial x_{\beta}} - p' \frac{\partial u_{\beta}^{"}}{\partial x_{\beta}} - \frac{\partial}{\rho} \left( v \frac{\partial u_{\beta}^{"}}{\partial x_{\alpha}} \cdot \frac{\partial u_{\beta}^{"}}{\partial x_{\alpha}} \right)$$

$$-\frac{\partial}{\rho} \left[ \frac{v}{3} \left( \frac{\partial u_{k}^{"}}{\partial x_{\alpha}} \right)^{2} \right]$$

$$(4-10)$$

where

$$\widetilde{\mathbf{u}_{\alpha}\mathbf{u}_{\beta}^{\mu}} = -\nu_{t} \left(\widetilde{\mathbf{k}}, \widetilde{\epsilon}\right) \left(\frac{\partial \widetilde{\mathbf{u}_{\alpha}}}{\partial \mathbf{x}_{\beta}} + \frac{\partial \widetilde{\mathbf{u}_{\beta}}}{\partial \mathbf{x}_{\alpha}}\right) \tag{4-11}$$

$$\frac{1}{2} \underbrace{u_{\alpha}'' u_{\beta}'' u_{\beta}''}_{2} + \frac{1}{2} \underbrace{p' u_{\alpha}''}_{\rho} = -\frac{v_{t}}{Sc_{t,k}} \frac{\partial \tilde{k}}{\partial x_{\alpha}}$$
(4-12)

$$-\frac{\overline{u_{\alpha}''}}{\overline{u_{\alpha}''}}\frac{\partial \overline{P}}{\partial x_{\alpha}} = \frac{T_{ad} - T_{o}}{\widetilde{T}} \underbrace{u_{\alpha}''_{s}}^{"} \frac{\partial \overline{P}}{\partial x_{\alpha}}$$
(4-13)

and  $Sc_{t,k}$  is the turbulent Schmidt number which is not species dependent and is chosen to be 0.9 in Equation (4-12).

Modified Dissipation Rate Equation of Turbulence:

$$\frac{\partial}{\partial t} \frac{\partial}{\rho \tilde{\epsilon}} + \frac{\partial}{\partial x_{\alpha}} \left( \frac{\partial}{\rho} \widetilde{u_{\alpha}} \widetilde{\epsilon} \right) = \frac{\partial}{\partial x_{\alpha}} \left( \frac{\partial}{\rho} \frac{v_{t}}{sc_{t,\epsilon}} \frac{\partial \widetilde{\epsilon}}{\partial x_{\alpha}} \right) - \frac{\partial}{\rho} C_{\epsilon 1} \left( \frac{\widetilde{u_{\alpha} u_{\beta}}}{u_{\alpha} u_{\beta}} \frac{\partial \widetilde{u_{\alpha}}}{\partial x_{\beta}} \right) - C_{\epsilon 1} \widetilde{u_{\alpha} u_{\beta}} \frac{\partial \widetilde{u_{\alpha}}}{\partial x_{\beta}} + C_{\epsilon 3} \widetilde{\widetilde{\epsilon}} \left( \frac{T_{ad} - T_{0}}{\widetilde{T}} \right) \widetilde{u_{\alpha} Y_{s}} \frac{\partial \overline{P}}{\partial x_{\alpha}} - \frac{\partial}{\rho} C_{\epsilon 2} \widetilde{\widetilde{\epsilon}} \frac{\widetilde{\epsilon}^{2}}{\widetilde{k}}$$

$$(4-14)$$

where  $Sc_{t,\epsilon} = 1.3$ ; constants  $C_{\epsilon 1} = 1.45$ ,  $C_{\epsilon 2} = 1.9$ ,  $C_{\epsilon 3} = 2.18$  and  $C_{D} = 2.$   $T_{ad}$  is the adiabatic flame temperature and  $T_{o}$  is the mixture

temperature of fuel and oxidizer.

(E) Reynolds Stress/Flux Models

The  $\tilde{k}-\tilde{\epsilon}$  model is based on the eddy viscosity/diffusivity concept in which it is assumed that the eddy viscosity/diffusivity is isotropic. This means that various Reynolds stress  $u''_{\alpha}u''_{\beta}$  and diffusion fluxes  $u''_{\alpha}\phi''$  ( $\phi''$  is either  $Y_s''$  or h'') are all taking similar forms. This assumption is certainly not true for complex flows (Jones, 1980). To overcome this problem, transport equations for the various Reynolds stresses and scalar diffusion fluxes must be derived from the Navier-Stokes equations. These equations contain higher order correlations which have to be approximated by lower order correlations to obtain a deterministic set of equations. The application of a Reynolds stress/flux turbulence closure model is limited because, especially in flows with a large number of species, the number of equations to be solved is large.

Reynolds Stress Closure Models include a transport equation for Reynolds stresses, a transport equation for diffusion scalar fluxes, a kinetic energy equation and a kinetic energy dissipation equation. These equations are shown as follows (Kollmann and Vandromme, 1979; Jones, 1980; Borghi, 1988):

Transport Equation of Reynolds Stresses:

$$\frac{\partial}{\partial t} \left( \bigcap_{\rho} u_{\alpha} u_{\beta}^{\prime \prime \prime} \right) + \frac{\partial}{\partial x_{\alpha}} \left( \bigcap_{\rho} u_{k} u_{\alpha}^{\prime \prime \prime \prime \prime} \right) = P_{\alpha\beta} + \frac{\partial}{\partial x_{k}} \left[ C_{s} \bigcap_{\rho} \frac{\tilde{k}}{\tilde{\epsilon}} \cdot \left( C_{s} \bigcap_{\rho} \frac{\tilde{k}}{\tilde{\epsilon}} \cdot C_{s} \bigcap_{\rho} \frac{\tilde{k}}{\tilde{k}} \cap C_{s} \bigcap_{\rho} \frac{\tilde$$

$$-\frac{C_{2} + 8}{11} \underbrace{P_{\alpha\beta}}_{P_{\alpha\beta}} - \frac{6C_{2} + 4}{11} \underbrace{\left( \stackrel{\frown}{\rho} \underbrace{u_{\alpha}u_{\beta}^{"}} \frac{\partial}{\partial x_{k}} \underbrace{u_{k}} + \delta_{\alpha\beta} \underbrace{P_{k}} \right)}_{11}$$

$$-\frac{2 - 8C_{2}}{11} \underbrace{\left( \stackrel{\frown}{\rho} \underbrace{u_{\alpha}^{"}u_{k}^{"}} \frac{\partial}{\partial x_{\beta}} \underbrace{u_{k}} + \stackrel{\frown}{\rho} \underbrace{u_{\beta}^{"}u_{k}^{"}} \frac{\partial u_{k}}{\partial x_{\alpha}} \right) - \frac{30C_{2} - 2}{55}}_{55} .$$

$$\cdot \underbrace{\left( \frac{\partial u_{\alpha}}{\partial x_{\beta}} + \frac{\partial u_{\beta}}{\partial x_{\alpha}} \right) \stackrel{\frown}{\rho k}}_{\rho k} + \frac{40C_{2} + 12}{55} \underbrace{\delta_{\alpha\beta}}_{\delta \alpha\beta} \underbrace{\frac{\partial u_{k}}{\partial x_{k}} \stackrel{\frown}{\rho k}}_{\rho k} - \frac{2}{3} \underbrace{\tilde{\epsilon}}_{\delta \alpha\beta} \underbrace{\delta_{\alpha\beta}}_{\delta \alpha\beta}$$

$$(4-15)$$

where

$$\widetilde{P}_{\alpha\beta} = -\frac{1}{\rho} \underbrace{u_{\alpha} u_{k}^{"}}_{\alpha x_{k}} \underbrace{\frac{\partial \widetilde{u}_{\beta}}{\partial x_{k}}}_{-\frac{1}{\rho} \underbrace{u_{\beta} u_{k}^{"}}_{\alpha x_{k}} \underbrace{\frac{\partial \widetilde{u}_{\alpha}}{\partial x_{k}}}_{(4-16)}$$

$$\widetilde{P}_{k} = \frac{1}{2} \widetilde{P}_{\alpha \alpha} = -\frac{1}{\rho} \widetilde{u}_{\alpha}^{ii} u_{\beta}^{ii} \frac{\partial \widetilde{u}_{\alpha}}{\partial x_{\beta}}$$
(4-17)

C<sub>1</sub> and C<sub>2</sub> are constant.

Transport Equation for Diffusion Scalar Fluxes:

$$\frac{\partial}{\partial t} \left( \stackrel{\sim}{\rho} \stackrel{\sim}{u_{\alpha}} \stackrel{\sim}{\phi} \right) + \frac{\partial}{\partial x_{\beta}} \left( \stackrel{\sim}{\rho} \stackrel{\sim}{u_{\beta}} \stackrel{\sim}{u_{\alpha}} \stackrel{\sim}{\phi} \right) = - \rho \stackrel{\sim}{u_{\beta}} \stackrel{\sim}{\phi} \stackrel{\sim}{u_{\alpha}} \frac{\partial u_{\alpha}}{\partial x_{\beta}} - \stackrel{\sim}{\rho} \stackrel{\sim}{u_{\alpha}} \stackrel{\sim}{u_{\beta}} \stackrel{\sim}{\phi} \right) .$$

$$\cdot \frac{\partial \stackrel{\sim}{\phi}}{\partial x_{\beta}} + \frac{\partial}{\partial x_{\beta}} \left[ C_{s} \stackrel{\sim}{\rho} \stackrel{\sim}{\overline{k}} \left( \stackrel{\sim}{u_{\alpha}} \stackrel{\sim}{u_{\alpha}} \stackrel{\sim}{\psi} \right) + C_{\phi 2} \stackrel{\sim}{\rho} \stackrel{\sim}{\overline{k}} \left( \stackrel{\sim}{u_{\alpha}} \stackrel{\sim}{u_{\beta}} \stackrel{\sim}{\psi} \right) \stackrel{\sim}{\partial x_{\beta}} \right) .$$

$$- \stackrel{\sim}{\phi} \stackrel{\sim}{\eta} \stackrel{\sim}{\partial x_{\alpha}} - C_{\phi 1} \stackrel{\sim}{\rho} \stackrel{\sim}{\overline{k}} \stackrel{\sim}{u_{\alpha}} \stackrel{\sim}{\phi} + C_{\phi 2} \stackrel{\sim}{\rho} \stackrel{\sim}{\overline{k}} \left( \stackrel{\sim}{u_{\alpha}} \stackrel{\sim}{u_{\beta}} \stackrel{\sim}{\psi} \right) \stackrel{\sim}{\partial u_{\beta}} \stackrel{\sim}{\partial x_{\beta}} .$$

$$\cdot \stackrel{\sim}{u_{\beta}} \stackrel{\sim}{\phi} \stackrel{\sim}{u_{\beta}} \stackrel{\sim}{\phi} \stackrel{\sim}{u_{\alpha}} \stackrel{\sim}{\phi} \stackrel{\sim}{u_{\alpha}} \stackrel{\sim}{\phi} \stackrel{\sim}{\eta} \stackrel{\sim}{\psi} \stackrel{\sim}{\psi}$$

where

$$\phi = (Y_s, h)$$

$$\phi^{il} = (Y_s^{il}, h^{il})$$

$$s = \frac{1}{\rho} W_s$$

$$(4-19)$$

 $C_s$ ,  $C_{\phi 1}$  and  $C_{\phi 2}$  are constants.

Modeling Equation for Fluctuating Velocity Components:

$$\frac{\partial}{\partial t} \left( \stackrel{\square}{\rho} \stackrel{\square}{u_{\alpha}} \right) + \frac{\partial}{\partial x_{\beta}} \left( \stackrel{\square}{\rho} \stackrel{\square}{u_{\beta}} \stackrel{\square}{u_{\alpha}} \right) = - \stackrel{\square}{\rho} \stackrel{\square}{u_{\beta}} \frac{\partial u_{\alpha}}{\partial x_{\beta}} + \left[ \stackrel{\square}{u_{\alpha}} \stackrel{\square}{u_{\beta}} - C_{s} \stackrel{\widetilde{k}}{\overline{\epsilon}} \stackrel{\square}{u_{\alpha}} \stackrel{\square}{u_{\alpha}} \right]$$

$$\cdot \frac{\partial}{\partial x_{k}} - \stackrel{\square}{u_{\beta}} + \stackrel{\square}{u_{\beta}} \stackrel{\square}{u_{k}} \frac{\partial}{\partial x_{k}} - \stackrel{\square}{u_{\alpha}} \stackrel{\square}{u_{\alpha}} \right) \left[ \stackrel{\partial}{\partial \rho} + \frac{\partial}{\partial x_{\beta}} \left[ C_{s} \stackrel{\widetilde{k}}{\overline{\epsilon}} \stackrel{\square}{u_{\alpha}} \stackrel{\square}{u_{\alpha}} \right] \right]$$

$$\cdot \frac{\partial}{\partial x_{k}} - \stackrel{\square}{u_{\beta}} + \stackrel{\square}{u_{\beta}} \stackrel{\square}{u_{k}} \frac{\partial}{\partial x_{k}} - \stackrel{\square}{u_{\alpha}} \stackrel{\square}{u_{\alpha}} \right] - C_{1c} \stackrel{\widetilde{\epsilon}}{\overline{k}} - \stackrel{\square}{u_{\alpha}} + C_{2c} \stackrel{\widetilde{\epsilon}}{\overline{k}} \stackrel{\square}{\rho} \stackrel{\square}{u_{\beta}}$$

$$\cdot \left( \stackrel{\square}{u_{\alpha}} \stackrel{\square}{u_{\beta}} - \frac{2}{3} \delta_{\alpha\beta} \right) - C_{3c} \stackrel{\square}{\rho} \stackrel{\square}{u_{\beta}} \frac{\partial u_{\alpha}}{\partial x_{\beta}} - C_{4c} \stackrel{\square}{\rho} \stackrel{\square}{u_{\alpha}} \frac{\partial}{\partial x_{\beta}} \stackrel{\square}{\rho} \stackrel{\square}{u_{\beta}} \stackrel{\square}{u_{\beta}}$$

$$\cdot \left( \stackrel{\square}{u_{\alpha}} \stackrel{\square}{u_{\beta}} - \frac{2}{3} \delta_{\alpha\beta} \right) - C_{3c} \stackrel{\square}{\rho} \stackrel{\square}{u_{\beta}} \frac{\partial u_{\alpha}}{\partial x_{\beta}} - C_{4c} \stackrel{\square}{\rho} \stackrel{\square}{u_{\alpha}} \frac{\partial}{\partial x_{\beta}} \stackrel{\square}{\rho} \stackrel{\square}{u_{\beta}} \stackrel{\square}{u_{\beta}} \stackrel{\square}{\alpha} \stackrel{$$

where  $C_s$ ,  $C_{1c}$ ,  $C_{2c}$ ,  $C_{3c}$ , and  $C_{4c}$  are constants.

Turbulent Kinetic Energy Equation:

$$\frac{\partial}{\partial t} (\vec{\rho}\vec{k}) + \frac{\partial}{\partial x_{B}} (\vec{\rho} \vec{u}_{B}\vec{k}) = P_{k} + \frac{\partial}{\partial x_{B}} \left[ C_{s} \frac{\vec{k}}{\vec{\epsilon}} - \frac{\vec{u}_{B}\vec{u}_{k}}{u_{B}\vec{u}_{k}} \frac{\partial \vec{k}}{\partial x_{k}} \right] - \frac{\vec{u}_{\alpha}}{u_{\alpha}} \frac{\partial \vec{P}}{\partial x_{\alpha}}$$

$$- \frac{\vec{\rho}\vec{\epsilon}}{(4-21)}$$

where  $P_k$  is shown in Equation (4-18), and  $C_s$  is a constant. Turbulent Kinetic Energy Dissipation Equation:

$$\frac{\partial}{\partial t} \left( \stackrel{\sim}{\rho \epsilon} \right) + \frac{\partial}{\partial x_{\beta}} \left( \stackrel{\sim}{\rho} \stackrel{\sim}{u_{\beta}} \stackrel{\sim}{\epsilon} \right) = C_{\epsilon 1} \frac{\tilde{\epsilon}}{\tilde{k}} \left( \stackrel{\sim}{P}_{k} - \stackrel{ii}{u_{\alpha}} \frac{\partial \overline{P}}{\partial x_{\alpha}} \right) + \frac{\partial}{\partial x_{\beta}} \cdot \left[ C_{\epsilon} - \stackrel{\sim}{\rho} \frac{\tilde{k}}{\tilde{k}} \stackrel{ii''}{u_{\alpha}} \stackrel{ii'}{u_{\beta}} \stackrel{ii''}{\partial x_{\alpha}} \right] - C_{\epsilon 2} - \stackrel{\sim}{\rho} \frac{\tilde{\epsilon}^{2}}{\tilde{k}}$$

$$(4-22)$$

## (F) Algebraic Stress/Flux Models

The Reynolds stress/flux model discussed in Section (4-E) is one of the most general turbulence closure models that can be applied to almost all kinds of turbulent flows. Disadvantages of this method, however, are the large number of differential equations that have to be solved and the complexity of the model. To overcome these problems, Algebraic Stress Models have been developed in which the transport equations for Reynolds stresses and diffusion scalar fluxes are simplified to algebraic equations, whereby the model still retains most of its basic features, such as for instance the anisotropic eddy viscosity/diffusivity concept (Rodi, 1976).

Transport Equation for Reynolds Stresses in Algebraic Expression:

$$\widetilde{u_{\alpha}^{"}u_{\beta}^{"}} = \frac{\widetilde{k}}{\left(\widetilde{P_{k}} + \widetilde{u_{\alpha}^{"}} \frac{\partial \overline{P}}{\partial x_{\alpha}} - \widetilde{\rho} \, \widetilde{\epsilon}\right)} \left\{\widetilde{P_{\alpha\beta}} - c_{1} \, \widetilde{\rho} \, \frac{\widetilde{\epsilon}}{\widetilde{k}} \, (\widetilde{u_{\alpha}^{"}u_{\beta}^{"}})\right\} \\
- \frac{2}{3} \, \delta_{\alpha\beta} \, \widetilde{k}) \, - \frac{C_{2} + 8}{11} \, \widetilde{P_{\alpha\beta}} - \frac{6C_{2} + 4}{11} \, \left(\widetilde{\rho} \, \widetilde{u_{\alpha}^{"}u_{\beta}^{"}} \, \frac{\partial \widetilde{u_{k}}}{\partial x_{k}}\right) \\
+ \, \delta_{\alpha\beta} \, \widetilde{P_{k}}\right) \, - \frac{2 - 8C_{2}}{11} \, \left(\widetilde{\rho} \, \widetilde{u_{\alpha}^{"}u_{k}^{"}} \, \frac{\partial \widetilde{u_{k}}}{\partial x_{\beta}} + \widetilde{\rho} \, \widetilde{u_{\beta}^{"}u_{k}^{"}} \, \frac{\partial \widetilde{u_{k}}}{\partial x_{\alpha}}\right) \\
- \frac{30C_{2} - 2}{55} \left(\widetilde{\partial u_{\alpha}^{"}} + \frac{\partial \widetilde{u_{\beta}}}{\partial x_{\beta}} + \frac{\partial \widetilde{u_{\beta}}}{\partial x_{\alpha}}\right) \, \widetilde{\rho} \, \widetilde{k} + \frac{40C_{2} + 12}{55} \, \delta_{\alpha\beta} \, \frac{\partial \widetilde{u_{k}}}{\partial x_{k}} \, \widetilde{\rho} \, \widetilde{k} + \frac{2}{3} \, \widetilde{\epsilon} \, \delta_{\alpha\beta}\right\}$$

$$(4-23)$$

where C<sub>1</sub> and C<sub>2</sub> are the constants.

Transport Equation for Diffusion Scalar Fluxes in Algebraic Expression:

$$\frac{\widetilde{u_{\alpha}^{"}}\phi^{"}}{\widetilde{v_{\alpha}^{"}}\phi^{"}} = \frac{2\widetilde{k}}{\left(\bigcap_{k} - \overline{u_{\alpha}^{"}} \frac{\partial \overline{p}}{\partial x_{\alpha}} - \rho \widetilde{\epsilon}\right)} \left\{ - \frac{\widetilde{u_{\beta}^{"}}\phi^{"}}{\widetilde{u_{\beta}^{"}}\phi^{"}} \frac{\partial \widetilde{u_{\alpha}}}{\partial x_{\beta}} - \frac{\widetilde{o_{\alpha}^{"}}u_{\alpha}^{"}u_{\beta}^{"}}{\partial x_{\beta}} + \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\partial \overline{p}}{\partial x_{\beta}} - \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\partial \overline{p}}{\partial x_{\beta}} + \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\partial \widetilde{u_{\alpha}^{"}}}{\widetilde{k}} - \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\partial \widetilde{u_{\alpha}^{"}}}{\widetilde{k}} - \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\partial \widetilde{u_{\alpha}^{"}}}{\widetilde{k}} - \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\partial \widetilde{u_{\alpha}^{"}}}{\widetilde{k}} - \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\partial \widetilde{u_{\alpha}^{"}}}{\widetilde{k}} + \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\partial \widetilde{u_{\alpha}^{"}}}{\widetilde{k}} + \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\partial \widetilde{u_{\alpha}^{"}}}{\widetilde{k}} - \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\partial \widetilde{u_{\alpha}^{"}}}{\widetilde{k}} + \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\partial \widetilde{u_{\alpha}^{"}}}{\widetilde{k}} + \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} + \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} - \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} + \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} + \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} \frac{\widetilde{o_{\alpha}^{"}}}{\widetilde{k}} + \frac{\widetilde{o_{\alpha}^{"}}}$$

where  $C_{\phi 1}$  and  $C_{\phi 2}$  are constants.

Modeling Equation for Fluctuating Velocity Components:

$$-\frac{1}{\rho} \frac{1}{u_{B}^{"}} \frac{\partial \widetilde{u}_{\alpha}}{\partial x_{B}} + \frac{1}{u_{\alpha}^{"} u_{B}^{"}} \frac{\partial \overline{P}}{\partial x_{B}} - C_{1c} \frac{\widetilde{\epsilon}}{\widetilde{\kappa}} - \frac{1}{u_{\alpha}^{"}} + C_{2c} \frac{\widetilde{\epsilon}}{\widetilde{\kappa}} - \frac{1}{u_{B}^{"}} \left( \frac{u_{\alpha}^{"} u_{B}^{"}}{\widetilde{\kappa}} - \frac{2}{3} \delta_{\alpha \beta} \right) + \\ -C_{3c} \frac{1}{\rho} \frac{\widetilde{u}_{\alpha}}{u_{B}^{"}} \frac{\partial \widetilde{u}_{\alpha}}{\partial u_{B}} - C_{4c} \frac{\overline{\rho^{2} u_{\alpha}^{"}}}{\overline{\rho^{2}}} \frac{\partial}{\partial x_{B}} \left( -\frac{\overline{u}_{\alpha}^{"}}{u_{B}^{"}} \right) = 0$$

$$(4-25)$$

where  $C_{1c}$ ,  $C_{2c}$ ,  $C_{3c}$  and  $C_{4c}$  are constants.

# (G) Multiple-Scale Turbulence Models

Turbulence consists of fluctuation motions with a continuous spectrum of length and time scales. The largest length scale of eddies have the dimension of the flow field, while the smallest length scales are related to the diffusive action of the molecular viscosity (Tennekes and Lumley, 1972). Turbulent energy production is related to the largest eddies, while dissipation of the turbulent energy is primarily related to the smallest eddies. Turbulence closure models which employ just a single length scale, therefore, are very

simplistic because they neglect the fact that production and dissipation of turbulent energy occur at different length scales. The fact that single-scale models yield successful predictions of many flow fields reflects more that these flows are close to spectral In other words, the production of turbulent energy of the large eddies  $(\epsilon_p)$  equals the dissipation of the small eddies  $(\epsilon_1)$ , namely  $\epsilon_p = \epsilon_T = \epsilon$ , rather than that the single-scale model is adequate (Hanjalic et al., 1980). In view of turbulent energy production occurring at large length scales and dissipation of turbulent energy mainly taking place at small length scales, there must be a transfer region of length scales in which turbulent energy is transferred from the largest eddies to the smallest. This transfer can introduce a lag phenomenon, namely turbulent energy production and turbulent energy dissipation do not both decrease or increase in the same regions of the flow (see Figure 1 for details), as for instance the  $\tilde{k}$ -  $\tilde{\epsilon}$  model implies (Hanjalic, et al., 1980). Figure 1 shows the energy spectral density of turbulence in a shear flow at high Reynolds number as a function of the wave number K (1/K is proportional to the length scale).

To introduce a model which takes into account the different processes at different length scales (or wave number), Hanjalic et al. (1980) divided the energy spectral density distribution into three parts, as shown in Figure 1. They assume that production of turbulent energy takes place at wave numbers below  $K_1$ , characterized by kinetic energy  $k_p$  and energy dissipation  $\epsilon_p$ , that transfer of turbulent energy takes place in the wave number range from  $K_1$  to  $K_2$ , characterized by kinetic energy  $k_1$  and energy dissipation  $\epsilon_1$  and that at wave numbers

division of the energy spectral density distribution into more than three parts is the key feature of the multi-scale-model. The energy spectral density range may be divided into as many parts as possible. In practice however, a division into three regions appears to be sufficient (Fabris et al., 1981). This requires two sets of transport equations. The  $\tilde{k}-\tilde{\epsilon}$  equations for the production region ( $K<\infty$ ) can be written as follows:

Kinetic Energy Equation for Production Region (K < K<sub>1</sub>):

$$\frac{\partial}{\partial t} \left( \stackrel{\frown}{\rho} \stackrel{\frown}{k_{p}} \right) + \frac{\partial}{\partial x_{B}} \left( \stackrel{\frown}{\rho} \stackrel{\frown}{u_{B}} \stackrel{\frown}{k_{p}} \right) = P_{k} - \frac{\mu_{t}}{Pr_{t} \stackrel{\frown}{\rho^{2}}} \frac{\partial \stackrel{\frown}{P}}{\partial x_{\alpha}} \frac{\partial \stackrel{\frown}{\rho}}{\partial x_{\alpha}} + \frac{\partial}{\partial x_{\beta}} \left[ \frac{\mu_{t}}{Pr_{t}} \frac{\partial \stackrel{\frown}{k_{p}}}{\partial x_{\beta}} \right] - \stackrel{\frown}{\rho} \stackrel{\frown}{\epsilon_{p}}$$

$$(4-26)$$

Energy Dissipation Equation for Production Region ( $K < K_1$ ):

$$\frac{\partial}{\partial t} \left( \stackrel{\sim}{\rho} \stackrel{\sim}{\epsilon_{p}} \right) + \frac{\partial}{\partial x_{\beta}} \left( \stackrel{\sim}{\rho} \stackrel{\sim}{u_{\beta}} \stackrel{\sim}{\epsilon_{p}} \right) = C_{p1} \frac{\widehat{\epsilon_{p}}}{\widehat{k_{p}}} \stackrel{\sim}{P_{k}} - C_{p1} \frac{\widehat{\epsilon_{p}}}{\widehat{k_{p}}} \frac{\mu_{t}}{\overline{\rho^{2}} Pr_{t}} \frac{\partial \overline{\rho}}{\partial x_{\alpha}} \frac{\partial \overline{P}}{\partial x_{\alpha}} + \frac{\partial}{\partial x_{\beta}} \left[ \frac{\mu_{t}}{Pr_{t}} \frac{\partial \stackrel{\sim}{\epsilon_{p}}}{\partial x_{\beta}} \right] - C_{p2} \stackrel{\sim}{\rho} \frac{\widehat{\epsilon_{p}}^{2}}{\widehat{k_{p}}}$$

$$(4-27)$$

where  $P_k$  is shown in Equation (4-18) and  $C_{p1}$  and  $C_{p2}$  are constants.

The  $\tilde{k}-\tilde{\epsilon}$  equation for the transfer region  $(K_2>K>K_1)$  can be shown as follows:

Kinetic Energy Equation for the Transfer Region  $(K_2 > K > K_1)$ :

$$\frac{\partial}{\partial t} \left( \stackrel{\sim}{\rho} \stackrel{\sim}{k_T} \right) + \frac{\partial}{\partial x_B} \left( \stackrel{\sim}{\rho} \stackrel{\sim}{u_B} \stackrel{\sim}{k_T} \right) = \stackrel{\sim}{\rho} \stackrel{\leftarrow}{\epsilon_p} + \frac{\partial}{\partial x_B} \left[ \frac{\mu_t}{Pr_t} \frac{\partial k_T}{\partial x_B} \right] - \stackrel{\sim}{\rho} \stackrel{\leftarrow}{\epsilon_T} (4-28)$$

Energy Dissipation Equation for the Transfer Region ( $K_2 > K_1$ ):

$$\frac{\partial}{\partial t} \left( \stackrel{\sim}{\rho} \stackrel{\sim}{\epsilon_{T}} \right) + \frac{\partial}{\partial x_{\beta}} \left( \stackrel{\sim}{\rho} \stackrel{\sim}{u_{\beta}} \stackrel{\sim}{\epsilon_{T}} \right) = C_{T1} \frac{\epsilon_{T}}{k_{T}} \stackrel{\sim}{\rho} \stackrel{\sim}{\epsilon_{p}} + \frac{\partial}{\partial x_{\beta}} \left[ \frac{u_{t}}{Pr_{t}} \frac{\partial \stackrel{\sim}{\epsilon_{T}}}{\partial x_{\beta}} \right] + C_{T2} \stackrel{\sim}{\rho} \frac{\stackrel{\sim}{\epsilon_{T}}^{2}}{k_{T}}$$

$$(4-29)$$

where

$$v_{t} = c_{\mu} \widetilde{k} \frac{\widetilde{k_{p}}}{\widetilde{\epsilon_{p}}} = c_{\mu} (\widetilde{k_{p}} + \widetilde{k_{T}}) \frac{\widetilde{k_{p}}}{\widetilde{\epsilon_{p}}}$$
 (4-30)

and  $Pr_t$ ,  $C_{T1}$  and  $C_{T2}$  are constants.

### V Model-Free Simulations of Turbulent Reacting Flows

In some cases, the approach based on turbulence models has been very successful, and the results obtained by such models have shown encouraging agreement in comparison with experimental data. In complex chemically reacting flow, however, modeling is extremely difficult because of the lack of knowledge of the intricate flow dynamics. Also, a turbulence closure optimized for a particular type of flow may not be adequate for predicting the flow behavior in other configurations. Moreover, since most of the interesting dynamical behavior of a flow is modeled a priori, the outcome of numerical computations based on these turbulence models cannot substantially advance our understanding of turbulent reacting flows (Givi, 1989).

Recently, improved efficiency of numerics, storage capability, and computational speed have made it possible to solve appropriate transport equations of turbulent flows directly, without the need for modeling over some limited parameter range (Givi, 1989). Such simulations (defined as Model-Free), in comparison with calculations utilizing turbulence models, have the advantage that the physics of the problem is not modeled, but is recovered directly from the computed results. The results can be further used to understand many important mechanisms of turbulent transport and their direct coupling with chemical reactions.

Model-free simulations consist of solving the time development of the detailed, unsteady structures in a turbulent flow field. The nonlinear transport equations are solved by means of very accurate numerical methods so that no averaging (Reynolds or Favre average) is necessary. Therefore, no turbulence modeling is required. In these simulations, data acquisition and statistical sampling of the ensemble data are performed by a procedure analogous to laboratory experiments. In this respect, the model-free simulations offer the advantage that the thermo-fluid parameters of the flow field can be easily varied, and the conditions of the numerical simulations are more controllable than those in the laboratory experiments (Givi, 1989).

The majority of the approaches in model-free simulations can be classified into two general sub-categories: (1) Direct Numerical Simulations (DNS), and (2) Large Eddy Simulations (LES).

#### (A) Direct Numerical Simulations

The main outcome of direct numerical simulations is the emergence of various numerical methods that are able to handle large variations of length and time scales within a turbulent flow field. The numerical schemes currently in use for direct numerical simulations of reacting turbulent flows can be classified into three categories: (1) Spectral and pseudospectral methods (Canuto et al., 1987; Anderson et al., 1984), (2) Lagrangian scheme (Oran and Boris, 1987) and (3) Finite difference methods (Davis and Moore, 1985).

Despite the capability of present day supercomputers in allowing the calculations with more than one million grid points, the range of length and time scales that can be resolved by direct numerical simulations is substantially smaller than those of turbulent flows of practical interest. This limits the applications of direct

numerical simulations to basic research problems in which the scales of the excited modes remain within the band of computationally resolved grids (either in physical or spectral domain). In practice this implies that for an accurate simulation, the magnitude of viscosity and diffusivity must be large enough to damp out the unresolved scales, and the magnitude of the computational time step must be kept small enough to capture the correct temporal evolution of the flow. These restrictions impose severe limitations for practical engineering applications.

#### (B) Large Eddy Simulations

The methodology of large eddy simulations involves the prefiltering of the transport equation by decomposing the transport variables into large-scale and sub-grid-scale components. The former component is related to the large eddies in the turbulent field, whereas the latter is the component containing the smallscale fluctuations (Schumann and Friedrich, 1986; 1987).

The pre-filtering of the variable  $\phi$  ( $x_{\alpha}$ , t) is performed by means of the convolution integral

$$\langle \phi (x_i, t) \rangle = \iiint_{\Delta_i} F_t (x_\alpha - x_{\alpha'}) \phi (x_{\alpha'}, t) dx_{\alpha'}$$
 (5-1)

where  $F_t$  is an appropriate filter function with a characteristic length along  $\alpha$ -direction,  $\Delta_{\alpha}$ ; <> represents the filtered variable; and the integration is over the entire flow field. The remaining portion of  $\phi$  from the filtered quantity is defined as the sub-grid-scale field, and is represented by

$$\phi'(x_{\alpha}, t) = \phi(x_{\alpha}, t) - \langle \phi(x_{\alpha}, t) \rangle$$
 (5-2)

The Large Eddy Simulation is a combination of the direct numerical simulation for the filtered portion of the transport variable <\$>>\$>\$, and the sub-grid-scale modeling of the small-scale component \$\$'\$. At first glance, the methodology seems similar to the familiar Reynolds averaging. A closer comparison between the two averaging procedures, however, indicates the superiority of the prefiltering method in that only the contribution of the small scale structures need to be modeled, whereas in Reynolds type averaging closures are needed for all the length scales of motion (Givi, 1989). The fact that the small scales of turbulence exhibit a more universal character is the main reason to believe that attempting to provide a subgrid scale model would be more promising than the previously followed procedures based on Reynolds averaging closures.

An obvious extension of this approach would involve solving a transport equation for density-weighted probability functions of the subgrid scalars rather than assuming their form. This approach, like its counterpart in turbulence modeling, has the advantage that the effect of the chemical reations (scalar-scalar correlations) will appear in the closed-form. However, models are needed for molecular diffusion within the subgrid.

The rate of progress in this area of direct numerical simulations depends on the advance in the fields of (a) numerical methods, (b) supercomputer technology, and (c) the mathematical description of reactive flow transport. Forseeable developments of advanced computational facilities, however, will not be sufficient to relax

the restriction of Direct Numerical Simulations to flows having small to moderate variations of the characteristic length and time scales (Givi, 1989; 1990). Hence, the boundaries of applicability of Direct Numerical Simulations are, and will continue to be, significantly restricted.

#### VI Turbulence Model Recommendation

As we have already mentioned, the diffusion fluxes require specification for the closure problem. It has been shown by the Boussinesq model, that the eddy viscosity,  $v_{\rm t}$ , is not a property of the fluid, but instead a function of a length and time scale. Also the length scales evolve from inhomogeneous large eddy integral length scales, through Taylor microscale, to homogeneous small eddy Kolmogoroff length scale before viscous dissipation effects turbulent energy dissipation.

In the turbulence modeling of the diffusion fluxes, such as  $u_{\alpha}^{"}u_{\beta}^{"}$ ,  $u_{\alpha}^{"}Y_{\epsilon}^{"}$  and  $u_{\alpha}^{"}h_{\epsilon}^{"}$ , through Boussinesq's eddy viscosity model, there are zero equation, one equation, two equation, modified two equation models, etc. These models are based on the assumption of isotropic turbulence in which the viscous dissipation of turbulent motion is simply given by the following expression:

$$\tilde{\epsilon} = \nu \left( \frac{\partial u_{\alpha}^{l_{1}}}{\partial x_{\beta}} \right)^{2}$$
 (6-1)

In other words, various Reynolds stresses and diffusion fluxes of turbulence take similar forms. This assumption is certainly not true for complex flows (Jones, 1980). To overcome this problem, transport equations for various Reynolds stresses and scalar diffusion fluxes must be derived from the Navier-Stokes equations. The Reynolds stress closure models include a transport equation for Reynolds stresses, a transport equation for diffusion scalar fluxes, a kinetic energy equation, and a kinetic energy dissipation equation. The

Reynolds stress/flux model is one of the most general turbulence closure models that can be applied to almost all kinds of turbulent flows. Disadvantages of this method, however, are the large number of differential equations that have to be solved and the complexity of the model. To overcome these problems, algebraic stress models have been developed in which the transport equations for Reynolds stresses and diffusion scalar fluxes are simplified to algebraic equations, whereby the model still retains most of its basic features, such as for instance the anisotropic eddy viscosity/diffusivity concept. However, this model has been hardly tested in combustion problems.

Turbulence consists of fluctuation motions with a continuous spectrum of length and time scales. The largest length scale of eddies have the dimension of the flow field, while the smallest length scales are related to the diffusive action of the molecular viscosity (Tennekes and Lumley, 1972). Turbulent energy production is related to the largest eddies, while dissipation of the turbulent energy is primarily related to the smallest eddies. The fact that single-scale models, employed by turbulence closure models, yield successful predictions of many flow fields, reflects more than that these flows are close to spectral equilibrium. In other words, the dissipation of turbulent energy of the large eddies equals the dissipation of the small eddies rather than that the single-scale model is adequate (Hanjalic et al., 1980). Multiple-scale turbulence models were introduced to take into account the different processes at different length scales which includes a transfer region of length scales in which turbulent energy is transferred from the largest eddies to the smallest. However, this model has not been tested to treat combustion problems.

In some cases, the results obtained by turbulence models have been very successful in comparison with experimental data. complex chemically reacting flows, however, modeling is extremely difficult because of lack of knowledge of the intricate flow dynamics. Also, a turbulence closure optimized for a particular type of flow may not be adequate for predicting the flow behavior in other configurations. To avoid these deficiencies caused by turbulence modeling, it is suggested to solve appropriate transport equations of turbulent flows directly, without the need for modeling over some limited parameter range. Model-free simulations have the advantage that the physics of the problem is not modeled, but instead taken from the computed results. Therefore, the results can be used to understand important mechanisms of turbulent transport and their chemical reactions. Direct numerical coupling with simulations and large eddy simulations are a large part of model-free Direct simulations are able to handle large variations simulations. of length and time scales in a turbulent flow field by the emergence of various numerical methods. Direct numerical simulations are limited to basic research problems rather than engineering applications because the range of length and time scales that can be resolved by direct numerical simulations is much smaller than those of turbulent flows

In this report, our major concerns were to examine how the available turbulence modelings or the methods of model-free direct

simulation of turbulence can be efficiently used for the practical engineering application in liquid rocket thrust chambers. With these major considerations in mind, the advantages and disadvantages of the available turbulence models are summarized below.

### (A) Zero Equation Models

These models assume isotropic turbulence, and can be applied to two-dimensional simple shear flows with mild pressure gradients, mild curvature with no flow seperation and/or rotation effects. They can be further applied to three-dimensional turbulent boundary layers with small cross flows and very mild pressure gradients without curvature and rotational effects. They are bad for turbulent flows with large cross flows; flows with curvature, rotation and separation; pressure and turbulence driven secondary flows; flows with abrupt changes in shear rate; shock induced separated flows, etc.

# (B) One Equation Models

Similar to zero equation models, these models assume isotropic turbulence, and can be applied to two dimensional simple shear flows without curvature and rotation effects. For the case of two dimensional separated flows in a diffuser, they are slightly better than the zero equation models. Disadvantages for these models are similar to those of the zero equation models.

## (C) Two Equation Models

These models have been widely tested with good results in combustion problems. However, the basic assumption of these models are still based on the isotropic eddy viscosity/diffusivity concept. This concept fails in complex flow problems.

(D) Two Equation Models Modified for Turbulent Combustion

Modification of two equation models can greatly improve the

quality of combustion modeling through the interaction of turbulent

flow and turbulent combustion. The following examples are given to

illustrate the modifications:

(D-1) Modification of Combustion Rate  $(\tilde{W})$ 

To find a model for the combustion rate  $\tilde{W}$  is at the core of the turbulent combustion modeling. The basic considerations of this modeling include: (1) The combustion rate  $(W_i)$ , given by chemical kinetics, is a molecular rate, and is a highly nonlinear function of several variables; and (2) Due to nonlinearity,  $\tilde{W}$  is a probability function for the encounter of combustion rates between various species and is not the value of  $W_i$  with the mean values of these variables only.

For a bi-molecular reaction between species A and B (A + B  $\rightarrow$  C) one obtains

$$W_A = W_B = -k_c Y_A Y_B \tag{6-2}$$

and then

$$W_{A} = -k_{c}Y_{A}Y_{B} = -k_{c}Y_{A}Y_{B} - k_{c}Y_{A}Y_{B}$$
 (6-3)

where  $k_c$  is a forward reaction rate constant. The following situations can exist, as shown below:

If  $Y_{A}$  and  $Y_{B}$  are fluctuating out of phase

$$\widetilde{Y_{A}^{"}Y_{B}^{"}} < 0 \Rightarrow \widetilde{Y_{A}Y_{B}} < \widetilde{Y}_{A}\widetilde{Y_{B}}$$

$$(6-4)$$

If  $Y_A$  and  $Y_B$  are fluctuating in phase

$$\widetilde{Y_{A}^{"}Y_{B}^{"}} > 0 \implies \widetilde{Y_{A}Y_{B}} > \widetilde{Y_{A}}\widetilde{Y_{B}}$$

$$(6-5)$$

If Y, and Y, prevent reaction

$$\widetilde{Y_A}Y_B = 0$$
 and  $\widetilde{Y_A} \neq 0$ ,  $\widetilde{Y_B} \neq 0$  (6-6)

The effect of temperature fluctuations could play an important role when the forward reaction constant  $k_c$  is a function of T, as in the case of combustion. Let us assume:

$$k_{c}(T) = k_{o} \exp\left(-\frac{T_{\lambda}}{T}\right)$$
 (6-7)

where  $k_0$  and  $T_{\lambda}$  are constants.

The mean reaction rate can be modeled with reference to an isothermal bimolecular reaction. For non-isothermal reactions, by using Equation (6-7) and expanding  $\exp(-T_{\lambda}/T)$  in a power series, we have mean values of the reaction rate shown as:

$$\widetilde{W}_{A} = \widetilde{W}_{B} = -k_{0}\widetilde{Y}_{A}\widetilde{Y}_{B} \exp\left(-\frac{T_{A}}{T}\right) \left[1 + \frac{Y_{A}^{h}Y_{B}^{h}}{\widetilde{Y}_{A}\widetilde{Y}_{B}} + P_{1}\left(\frac{T_{A}}{\widetilde{T}}\right) \left(\frac{Y_{A}^{h}T^{H}}{\widetilde{Y}_{A}\widetilde{T}} + \frac{Y_{B}^{H}T^{H}}{\widetilde{Y}_{B}\widetilde{T}}\right) + P_{2}\left(\frac{T_{A}}{\widetilde{T}}\right) \frac{T^{H}^{2}}{(\widetilde{T})^{2}} + P_{1}\left(\frac{T_{A}}{\widetilde{T}}\right) \left(\frac{T^{H}^{2}Y_{A}^{H}}{\widetilde{T}^{2}\widetilde{Y}_{A}} + \frac{T^{H}^{2}Y_{B}^{H}}{\widetilde{T}^{2}\widetilde{Y}_{B}}\right) + P_{3}\left(\frac{T_{A}}{\widetilde{T}}\right) \frac{T^{H}^{3}}{(\widetilde{T})^{3}} + \cdots\right]$$
(6-8)

where the terms  $P_i \ \left( \frac{T_{\lambda}}{\widetilde{T}} \right)$  are polynomials of  $\frac{T_{\lambda}}{\widetilde{T}}$  .

(D-2) Modification of Turbulent Diffusion Fluxes By Combustion Further modification of turbulent diffusion fluxes, shown in Equation (2-12), is needed for consideration of the influence of combustion on turbulence through the modification of the turbulent reaction rate. Turbulent diffusion fluxes  $u_{\alpha}Y_{i}$  modified by combustion can be shown as follows (Borghi and Dutoya, 1978; Borghi and Escudie, 1984; Launder, 1976):

$$\frac{\partial}{\partial t} - \widetilde{u_{\alpha}'}_{i}'' + \frac{\partial}{\partial x_{\beta}} (\overline{\rho} \ \widetilde{u_{\beta}'} \ \widetilde{u_{\alpha}'}_{i}'') = \frac{\partial}{\partial x_{\beta}} (-\overline{\rho} \ \widetilde{u_{\alpha}'}_{i}''_{i}'') 
+ \overline{P'Y_{i}''} \delta_{\alpha\beta}) - \overline{\rho} \ \widetilde{u_{\alpha}'}_{i}''_{i} \frac{\partial \widetilde{Y_{i}}}{\partial x_{\beta}} - \overline{\rho} \ \widetilde{u_{\beta}'}_{i}''_{i} \frac{\partial \widetilde{u_{\alpha}}}{\partial x_{\beta}} + \overline{P'} \frac{\partial Y_{i}''}{\partial x_{\alpha}} 
- \overline{Y_{i}''} \frac{\partial \overline{P}}{\partial x_{\alpha}} + \overline{\rho} \ \widetilde{u_{\alpha}'}_{i}''_{i}.$$
(6-9)

In this equation, the term  $\overline{Y}_i''$  remains because the fluctuation is a density weighted fluctuation (that is  $\overline{\rho Y}_i'' = 0$  and  $\overline{Y}_i'' \neq 0$ ).

### (E) Reynolds Stress/Flux Models

Boussinesq's eddy viscosity/diffustion fluxes models have been adopted in the turbulence closure modeling of zero equation, one equation, and two equation (including  $\tilde{k}-\tilde{\epsilon}$  model) models. According to Boussinesq's formulation, isotropic turbulence is a foundation in the turbulence modeling, but this is not true for complex flows (Jones, 1980; Givi, 1989). To overcome the unappropriate assumption of isotropic turbulence for the description of thrust chamber reacting flow problems, transport equations for the various Reynolds stresses  $u_{\alpha}^{"}u_{\beta}^{"}$ , and diffusion fluxes  $u_{\alpha}^{"}h'$  and  $u_{\alpha}^{"}Y_{i}^{"}$ , must be derived from the mean value balance equations of continuity, momentum, energy and species concentrations.

The advantages of adopting Reynolds stress/flux models in turbulent thrust chamber reacting flow problems are that they are applicable to almost all turbulent flow problems. There are some disadvantages for adopting this model which include: (1) a very large number of partial differential equations to be solved, especially for multi-component mixtures; (2) the mathematical

formulation of this model is very complex; and (3) model is hardly tested for combustion reacting flow problems.

With present day advances in supercomputer technology, the former two disadvantages quoted can be easily solved as the new generation hardware components and software techniques are developed. As to the last disadvantage quoted for the limited number of combustion reacting flow tests, it can be improved through the endeavor of joint controlled modeling-experiment efforts in reacting flow problems.

In this regard, we strongly recommend the Reynolds stress/flux model as a major candidate for the future study in thrust chamber turbulent reacting flow problems.

## (F) Algebraic Stress/Flux Models

To overcome the disadvantages of the large number of differential equations that have to be solved and the complexity of the mathematical models associated with Reynolds stress/flux models, algebraic models have been developed to simplify the transport equations for Reynolds stresses and diffusion scalar fluxes to algebraic equations (Rodi, 1976). The advantages of this model are that it is very general in nature, and simpler in mathematical forms than that of the Reynolds stress/flux models, but still retains the basic features, such as the non-isotropic eddy viscosity/diffusivity concepts. The disadvantages of this model are that it is still very complex mathematically in comparison with other models, such as  $\tilde{k}-\tilde{\epsilon}$  models, and it has been little tested with respect to combustion problems.

## (G) Multiple-Scale Turbulence Models

Length and time scale motions vary constantly in turbulenc. Although production and dissipation of turbulent energy occur at different length scales, turbulence closure models employ only a single length scale (Hanjalic et al., 1980). By introducing a turbulence model with different length scales, one can handle the turbulence energy spectral density distribution transition from smaller wave numbers (turbulence energy production) to larger wave numbers (turbulence energy dissipation).

The multiple-scale turbulence models can either be associated with eddy viscosity/eddy diffusion concept formulations or with Reynolds stress/flux type manipulation.

#### (H) Model-Free Simulations

Instead of seeking turbulence models based on Favre and Reynolds averages for obtaining mean values and correlation mean values of fluctuations for thermochemical and flow variables of chemically reacting flows, one can use a model-free simulation by solving the balance equations directly (Givi, 1989; 1990). These model-free simulations include Direct Numerical Simulations and Large Eddy Simulations.

The advances in the fields of model-free simulations are strongly dependent upon the mathematical description of reactive flow transport in addition to the progress in supercomputer technology and numerical methods. In other words, direct numerical simulations having small variations of characteristic length and time scales will still be restricted even with the development of advanced computer

facilities (Givi, 1989; 1990). Within a forseeable future, the applicability of direct numerical simulation to the turbulent reacting flow problems will be mainly in the academic interests, and will be significantly restricted for engineering applications.

#### VII. Conclusions

Turbulence is rotational and three-dimensional. Turbulence is characterized by high levels of fluctuating vorticity and random fluctuations in nature. Turbulent flows are always dissipative, while the random waves are essentially non-dissipative (Tennekes and Lumley, 1972). Turbulence is a continuum phenomenon, and even the smallest scales occurring in a turbulent flow are ordinarily far larger than any molecular length scale. Turbulence is not a feature of fluids but of fluid flows.

Thermochemical flow parameter and fluctuations of motions of length and time scales vary continuously in turbulence. This means a turbulent flow has to be considered as an ensemble of random flow fields. Indeed, only statistical quantities are of practical meaning in order to describe the randomness within the flow.

Turbulent reacting flow problems can be attacked either by model-free direct simulation approaches, or by the use of Favre and Reynolds averages for the ensemble of flow fields. Model-free simulations include Direct Numerical Simulations and Large Eddy Simulations. Model-free simulations will continue to be significantly restricted for engineering applications of turbulent reacting flow problems because the advancement of supercomputer technology and numerical methods alone can not solve the mathematical description of reactive flow transport arising from the nature of random fluctuations of turbulent flow fields (Givi, 1989; 1990). Table 1 shows the classifications of approach used to handle turbulent

flow problems including model-free simulation and turbulence modeling.

The other approach is to connsider the variations and fluctuations of fluid density, which are more likely to occur in reacting flows with large temperature differences in turbulent combustion studies, by using mean values weighted by the density to handle fluid flows with a nature of randomness, irregularity, diffusivity and dissipation. This type of approach can be further divided into two large groups, with and without considering the Boussinesq expression of closure assumption.

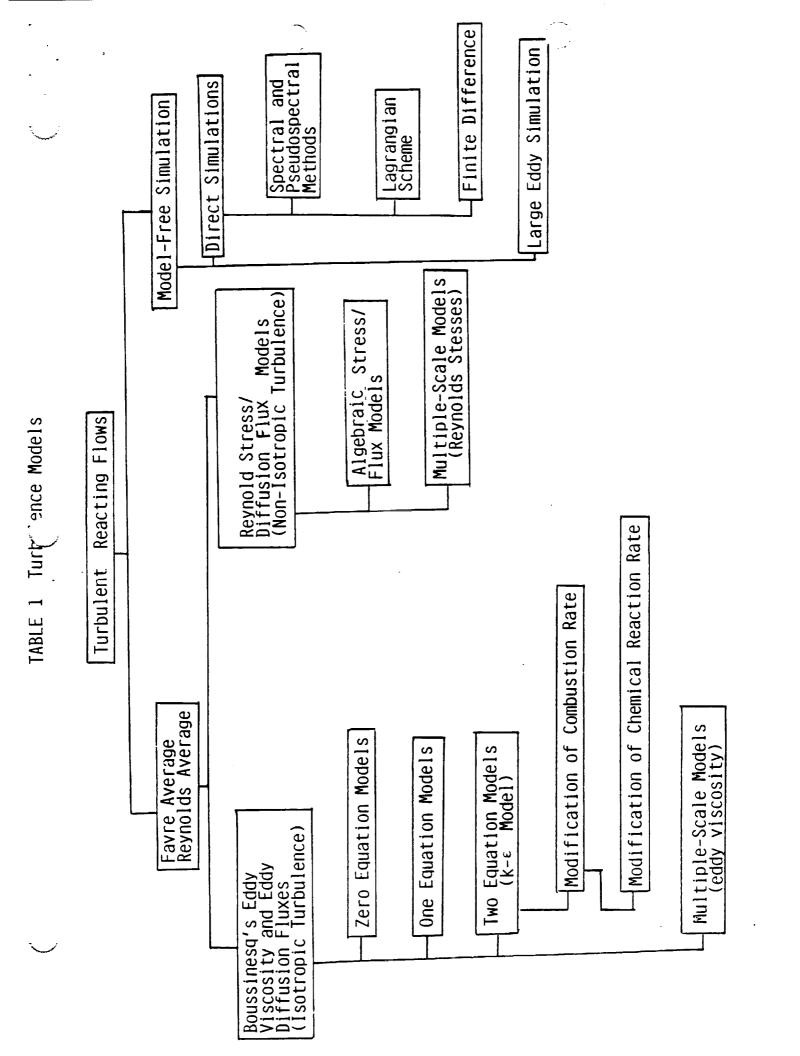
Turbulent reacting flow problems can not be solved by using mean balance equations of continuity, momentum, energy, and species concentration. These equations involve new quantities of the turbulent Reynold stress/diffusion fluxes. For example,  $u_{\alpha}^{"}u_{\beta}^{"}$ ,  $u_{\alpha}^{"}h_{\gamma}^{"}$  and  $u_{\alpha}^{"}Y_{i}^{"}$  are usually greater than the mean molecular scale, also correlations between fluctuations are not mean values only.

With adopting Boussinesq's expression of closure assumption, one can introduce the concepts of eddy viscosity/eddy diffusion fluxes. Turbulence modelings based on Boussinesq's expression include zero equation, one equation, two equation (this contains  $\tilde{k}-\tilde{\epsilon}$  models with and without modifications of combustion rate chemical reaction rate, etc.), and multiple-scale models associated with eddy viscosity. Most of the turbulence modelings based on Boussinesq's expression of closure assumptions have been widely used in engineering applications, and also widely tested with good results in combustion problems. However, the fundamentals of Boussinesq's

expression are built on the assumption of an isotropic eddy viscosity/diffusivity concept. This assumption is certainly not true for complex flows (Jones, 1980; Givi, 1989). In particular, the isotropic turbulence assumption fails in complex flow problems for the description of thrust chamber reacting flow fields.

Reynolds stress/flux models adopt the transport equations derived from the mean values balance equations of continuity, momentum, energy and species without using Boussinesq's expression of closure assumptions. This makes Reynolds stress/flux models very general and applicable to almost all flow problems. It is true that this model requires a large number of partial differential equations to be solved, especially for multi-component mixtures, in addition to formulation. With mathematical complexity its in advancement in supercomputer technology and numerical methods in the foreseeable future, we strongly recommend that the Reynolds stress/flux model be adopted as a major candidate in the future development of computation tools for the study of thrust chamber turbulent reacting flow problems.

A workshop was held on the campus of the University of Alabama in Huntsville during the time period of April 15 and 17, 1991, in connection with one task of a contract between the University and NASA Marshall Space Flight Center. The contractual effort was oriented to review various turbulence models, used in existing liquid rocket thrust chamber flow simulation programs, and other potential techniques. The study resulted in the recommendation of the Reynolds Stress Model.



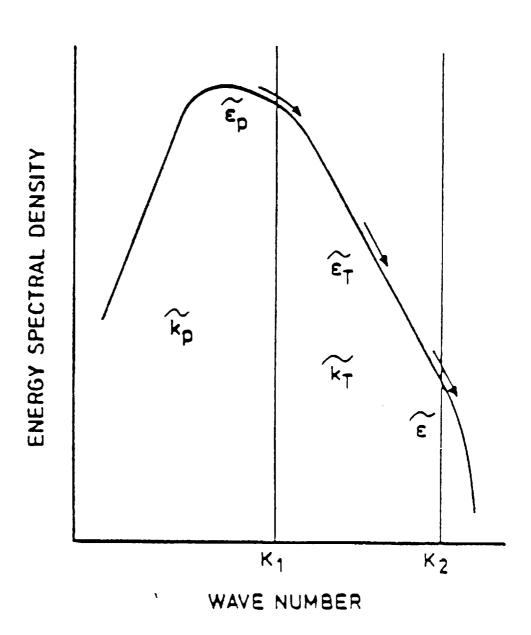


Figure 1 Spectral Division of Turbulent Energy and Dissipation Rate for Multiple-Scale Turbulence Modeling.

### Acknowledgement

The author appreciates the support received from the National Aeronautics and Space Administration through NASA Contract NAS8-36955/Delivery Order Number 38. He would like to express his gratitude to Klaus Gross of NASA/Marshall Space Flight Center for the stimulating discussions during the course of the present study.

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#### Appendix A

Conventional Mean Values (Reynolds Average)
and Density Weighted Mean Values (Favre Average) of
Turbulent Reacting Flows

Due to the variations and fluctuations of the fluid density which are more likely to occur in reacting flows with large temperature differences, it is rather common, in turbulent combustion studies, to change the classical definition of conventional mean values (Reynolds average) to density weighted mean values (Favre average). It appears that the use of mean values weighted by density is better able to handle fluid flows with randomness, diffusive and dissipative irregularity.

The conventional mean values are defined as:

$$A = \overline{A} + A' \tag{A-1}$$

where () is the conventional mean value and ()', the corresponding value for fluctuation. () can be further defined as:

$$\overline{A} = \lim_{t \to \infty} \frac{1}{2T} \int_{-T}^{T} Adt$$
 (A-2)

This formulation of conventional mean values can be written as

$$A(x_i, t, v) = \overline{A}(X_i, t) + A'(x_i, t, v)$$
 (A-3)

where:

$$\overline{A} (x_i, t) = \int_{-\infty}^{\infty} A (x_i, t, v) f(v) dv$$
 (A-4)

The function f(v) is the probability function of the property v. This function is defined such that f(v)dv is the probability that the value

of A at a fixed point  $(x_i, t)$  lies in the range from v to v + dv. Because v represents all possible values that A can take at a given point  $(x_i, t)$ , it is clear that:

$$\int_{-\infty}^{\infty} f(v) dv = 1$$
 (A-5)

The density weighted mean values are defined as:

$$A(x_i, t, v) = A(x_i, t) + A''(x_i, t, v)$$
 (A-6)

where () is the density-weighted mean value, and ()'' the corresponding value for fluctuations. () can be further defined as

$$\bigwedge_{A(x_i, t)} = \int_{-\infty}^{\infty} A(x_i, t, \nu) g_{\lambda}(\nu) d\nu$$
(A-7)

The function  $g_{\lambda}(\nu)$  is the density weighted probability density function of A. It is also clear that

$$\int_{-\infty}^{\infty} g_{\lambda}(\nu) d\nu = 1$$
 (A-8)

There are some close relations between conventional mean values and density-weighted mean values. Some useful relations are shown as follows:

$$\overline{\overline{A}} = \int_{-\infty}^{\infty} \overline{A}(x_i, t) f(v) dv = \overline{A} \int_{-\infty}^{\infty} f(v) dv = \overline{A}$$
(A-9)

$$\underbrace{\overline{A}}_{-\infty} = \int_{-\infty}^{\infty} \overline{A}(x_i, t) g_{\lambda}(\nu) d\nu = \overline{A} \int_{-\infty}^{\infty} g_{\lambda}(\nu) d\nu = \overline{A}$$
(A-10)

$$\widetilde{\widetilde{A}} = \int_{-\infty}^{\infty} A(x_i, t) g_{\lambda}(\nu) d\nu = A \int_{-\infty}^{\infty} g_{\lambda}(\nu) d\nu = \widetilde{A}$$
(A-11)

$$\overline{\widehat{A}} = \int_{-\infty}^{\infty} A(x_i, t) f(v) dv = A \int_{-\infty}^{\infty} f(v) dv = \widetilde{A}$$
 (A-12)

$$\overline{A} = \overline{\overline{A} + A'} = \overline{A} + \overline{A'} \Rightarrow \overline{A'} = 0 \tag{A-13}$$

$$\overline{A} = \overline{\widetilde{A} + A''} = \widetilde{A} + \overline{A''} \Rightarrow \overline{A''} \neq 0 \tag{A-14}$$

$$\overline{A} = \overline{\widetilde{A} + A''} = \widetilde{A} + \overline{A''} \Rightarrow \overline{A''} \neq 0$$

$$\widetilde{A} = \frac{\overline{\rho A}}{\overline{\rho}} = \frac{\overline{\rho A} + \rho' \overline{A} + \overline{\rho A'} + \rho' A'}{\overline{\rho}} = \frac{\overline{\rho A} + \rho' A'}{\overline{\rho}}$$

$$= \overline{A} + \frac{\overline{\rho' A'}}{\overline{\rho}} \tag{A-15}$$

mean values, of density-weighted equivalence conventional mean values, shown in the Equation (A-15), particularly important. To give an example, the continuity equation is

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_{\alpha}} (\rho u_{\alpha}) = 0 \tag{A-16}$$

In density-weighted mean values form the equation becomes

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_{\alpha}} (\overline{\rho} u_{\alpha}) = 0$$
 (A-17)

The equivalent conventional mean values form is

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_{\alpha}} \left( \overline{\rho} \ \overline{u_{\alpha}} + \overline{\rho' u_{\alpha'}} \right) = 0 \tag{A-18}$$

This means that the Favre-averaging continuity equation is simpler in form because it contains no terms involving density fluctuations.

In general, density weighted mean values apply velocity components  $(u_{\alpha})$ , temperature (T), mass fraction  $(Y_s)$  and enthalpy (h), while the conventional mean values are kept for pressure (P) and density  $(\rho)$ .